

1,1,1,3,3,3-Hexafluoro-2-propanol
920-66-1 | DTXSID1022134

Model Performance

Model	Data
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Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.56

Global applicability domain: Inside

Local applicability domain index: 5.22e-01

Confidence level: 7.54e-01

Nearest Neighbors from the Training Set

Image not found

1,1,1,3,3,3-Hexafluoro-2-propanol

Measured: 1.66
Predicted: 1.56

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N-Ethyl-2,2,2-trifluoroethan-1-amine

Measured: 0.74
Predicted: 8.54e-01

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Isoflurane
Measured: 2.06
Predicted: 2.08

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1-Propanol, 2,2,3,3,3-pentafluoro-

Measured: 1.23
Predicted: 1.14

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Ethyl trifluoroacetate

Measured: 1.18
Predicted: 1.04